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## 2-D mathematical modeling for a large electrochromic window—Part I

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## ABSTRACT

Electrochromic (EC) devices show a promise to be the next major advance in the energy-efficient window technology. However, the development of higher value (performance and cost) EC windows is the key to promote the applications of these energy saving devices. To that end, computer modeling may play a powerful role in providing in-depth understanding in EC device design, performance enhancement, material selection and development of EC layers. In this work, we describe a 2D time-dependent finite element based solver, established to simulate large area Li ion electrochromic devices. The results of 2D-model development and corresponding simulations are presented utilizing literature-based material properties. The capability of the model is demonstrated in handling a very large width-to-thickness aspect ratio and examining the impacts of a voltage change due to the spreading resistance and a diffusivity variation inside electrodes on device performance and lithium ion transport kinetics.

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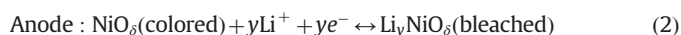
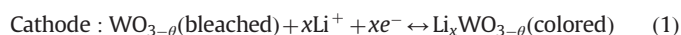
## 1. Introduction

Electrochromic (EC) windows have many advantages ranging from energy saving potential to human comfort in buildings [1]. Lee et al. pointed out that smart windows based on electrochromic switching principles were able to get total annual energy use savings up to 48% over conventional single-pane windows [2]. The EC technology could help achieve the US Department of Energy's goal of Net-Zero Energy buildings by reducing the energy liability of windows and skylights [3]. It has the potential of reducing peak electric loads by 20–30% in many commercial buildings and increasing day lighting benefits, as well as improving comfort and potentially enhancing productivity in our homes and offices. However, current electrochromic dynamic window products suffer from high cost and inadequate relative energy savings performance compared to low-E coated windows. The primary reason is the unavailability of a low cost process technology (equipment, deposition processes, integration, patterning, manufacturing, etc.) to fabricate the devices on large area architectural glass at high rate. While commercial glass coating technology is available, innovations are required to make the key active electrochromic layers compatible with high volume manufacturing and in materials that improve the energy savings. Therefore, developing fabrication methods, new materials and device configurations for low

cost and improved EC performance are the keys to promote the applications of these energy-saving devices.

Our major focus has been on increasing the value proposition, which is necessary for broad market applicability, by lowering manufacturing cost and improving device performance. To reach the above goals, computer modeling may play a powerful role in providing in-depth understanding in EC device design, performance enhancement, material selection and development of electrochromic layers [2,4].

In principle, an EC device as shown in Fig. 1 is able to change its optical properties as a response to an applied voltage. As illustrated in the reaction Eqs. (1) and (2), the change in optical properties of such a device results from electrochemical intercalation or extraction/de-intercalation of Li ions between the EC layer (e.g.,  $\text{WO}_{3-\theta}$ ) and the counter electrode (e.g.,  $\text{NiO}_\delta$ ), causing a color change:



Lithium insertion in the  $\text{WO}_{3-\theta}$  host, containing mainly  $\text{W}^{4+}$  and  $\text{W}^{6+}$  states, generates  $\text{W}^{5+}$  states which are responsible for coloration, as a result of the reduction of  $\text{W}^{6+}$  states. The optical absorption in the colored host is presumably caused by electronic transitions between the  $\text{W}^{6+}$  and  $\text{W}^{5+}$  and also between the  $\text{W}^{5+}$  and  $\text{W}^{4+}$  states [5–7]. In the  $\text{NiO}_\delta$  anode, there are two oxidation states:  $\text{Ni}^{2+}$  and  $\text{Ni}^{3+}$ .  $\text{Ni}^{2+}$  is colorless while  $\text{Ni}^{3+}$  shows a dark brown color.  $\text{Ni}^{3+}$  is reduced to  $\text{Ni}^{2+}$  by getting an electron during lithium intercalation and the film switches to its clear state. The film becomes dark brown when the reverse reaction happens [8]. Coloration of EC

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## Nomenclature

|             |  |                        |   |
|-------------|--|------------------------|---|
| $a_a$       | anodic empirical constant                            | $L_c$                  | cathode thickness                                   |
| $a_c$       | cathodic empirical constant                          | $L_{el}$               | separator thickness                                 |
| $c_i$       | concentration of $\text{Li}^+$ in electrode $i$      | $n$                    | number of participating electrons                   |
| $c_{max}^a$ | maximum concentration of anode                       | $R_i$                  | chemical reaction term in electrode surface         |
| $c_{max}^c$ | maximum concentration of cathode                     | $x$                    | lithium intercalation level in the cathode          |
| $D_a$       | diffusivity of anode                                 | $y$                    | lithium intercalation level in the anode            |
| $D_c$       | diffusivity of cathode                               | $\eta$                 | overpotential                                       |
| $D_{el}$    | diffusivity of electrolyte                           | $\phi_i$               | surface potential at the interface of electrode $i$ |
| $F$         | Faraday constant                                     | $\phi_l$               | surface potential at the interface of electrolyte   |
| $j_{loc}$   | local current density on the intercalation interface | $\nu$                  | stoichiometric coefficient                          |
| $L_a$       | anode thickness                                      | $\sigma_i \varepsilon$ | electrical conductivity of electrode $i$            |
|             |  | $\sigma_{il}$          | ionic conductivity of the electrolyte               |
|             |  | $U_i$                  | open circuit of electrode $i$ .                     |

devices is effectively able to block solar radiation and avoid uncomfortable brightness inside buildings.

In the past, many researchers focused on modeling cathode-related phenomena in EC devices. Nagai et al. studied lithium ion transport behavior in different electrochromic layers by refining a finite diffusion model [9]. Broclawick et al. proposed a cluster model for excitation process in solid tungsten oxide by using the density-functional theory approach, which provided results both for the electrically neutral cluster and for the cluster with an extra electron mimicking the effect of electron injection from the cathode [10]. Wang et al. generated a simulation model for ion injection and extraction under constant current conditions at  $\text{WO}_{3-\theta}$  electrodes and studied voltage–time curves, concentration profiles and surface concentration of lithium [11]. Based on the films constituted with nano-sized heterogeneous  $\text{WO}_3$  particles, pores and adsorbed substances, Lusiš et al. developed a model explaining the dependence of coloration characteristics on constitution, composition, atomic structure and size of  $\text{WO}_x$  particles [12]. Vuillemin and Bohnke described the mechanism of the EC process in a- $\text{WO}_3$  with a model based on the double injection of cations and electrons into the tungsten oxide, indicating that the kinetics of coloration was considered to be limited by the diffusion of the intermediate species into the oxide [13]. Fuller, Doyle et al. developed a general model to simulate and predict the galvanostatic charge and discharge of a lithium-ion cell [14–15], which in principle is very much similar to electrochromic devices [16], with a mixture of active insertion material, electrolyte and inert conducting material. Good agreement between simulation and experiment was observed.

Our work involves a 2-D mathematical model for an EC device with commonly used configuration to evaluate and predict kinetics of interfacial lithium intercalations and lithium diffusion inside cathode and anode, and device responses with material and

dimension changes. This paper, as the first part of two papers, focuses on the establishment of the numerical 2-D simulation model. Such a model is able to carry out time-dependent simulation for a large area full stack EC device. The capability of the modeling is demonstrated by predicting effects of material properties (open circuit potential (OCP), diffusion coefficient and spread resistance) on voltage variation and intercalation kinetics and the distribution of lithium ions inside the electrodes and at electrode/electrolyte interfaces. As an extension of this work, the upcoming Part II will provide the confirmation of the 2-D model with in-house generated data and prediction of EC responses to material property and device dimension variations in terms of uniformity and speed of lithium transport.

## 2. Simulation model

### 2.1. Model development

A typical film stack of an electrochromic device is shown in Fig. 1. In a bottom-up sequence, the bottom layer is a transparent conductive oxide (TCO). The second from the bottom is the cathode layer, followed by a solid state electrolyte layer such as lithium phosphorous oxynitride (LiPON) [17–18], which is a  $\text{Li}^+$  ion conductor and electronic insulator. On top of the LiPON layer is the anode layer covered by another TCO layer, serving as the counter current collector. Top left and bottom right are the connecting points to an external power supply. In this study, the 3D model shown in Fig. 1 is simplified to a 2D model, as shown in Fig. 2. The 2D model considers only the X-Z plane, where Z is perpendicular to the stacked layers and X is along the width of the device. The 2D model is sufficient in describing the behavior of lithium transport and intercalation in EC windows as the highly conductive electrical contacts of the current collectors run along the Y axis, providing equipotential lines.

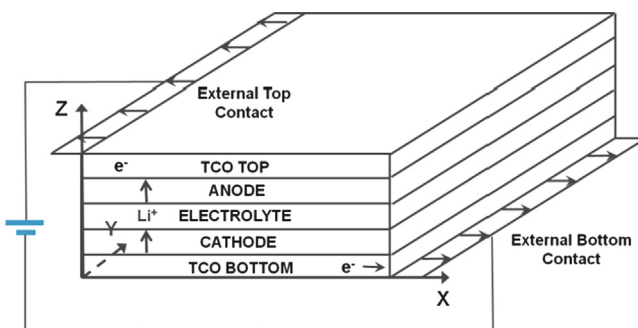


Fig. 1. A schematic diagram of a typical electrochromic device structure. Arrows indicate the movement of electrons out to the external circuit and Li ion internally for clearing reaction.

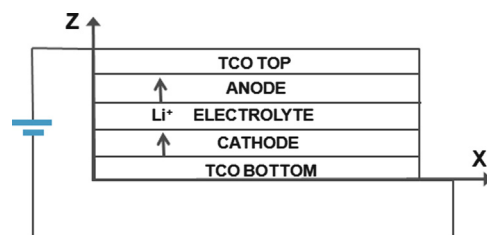


Fig. 2. Two-dimensional electrochromic simulation model.

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